

Replacement Pages for Claims 1-18

(CLEAN FORM)

1. A method for use in deriving fixed bond information, comprising:
analyzing a delocalized representation of a chemical structure;
identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
evaluating at least a subset of the fixed bond representation candidates; and
selecting from among the plurality of fixed bond representation candidates based on the evaluation.
2. A system for use in deriving fixed bond information, comprising:
an analyzer analyzing a delocalized representation of a chemical structure;
an identifier identifying, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
an evaluator evaluating at least a subset of the fixed bond representation candidates; and
a selector electing from among the plurality of fixed bond representation candidates based on the evaluation.
3. Computer software, residing on a computer-readable storage medium, comprising a set of instructions for use in a computer system to help cause the computer system to derive fixed bond information, the instructions causing the system to:
analyze a delocalized representation of a chemical structure;
identify, based on valence information, a plurality of fixed bond representation candidates for at least a portion of the chemical structure;
evaluate at least a subset of the fixed bond representation candidates; and
select from among the plurality of fixed bond representation candidates based on the evaluation.
4. The method of claim 1, wherein at least a portion of the delocalized representation describes a monocyclic ring system.
5. The method of claim 1, wherein at least a portion of the delocalized representation describes a polycyclic ring system.

6. The method of claim 1, wherein at least a portion of the delocalized representation describes a ring system with a hetero substitution pattern.

7. The method of claim 1, wherein at least a portion of the delocalized representation describes a non-cyclic system.

Sub 2 8. The method of claim 1, wherein at least a portion of the delocalized representation describes an incompletely cyclic system.

Sub 3 9. The method of claim 1, further comprising:
including, in the produced fixed bond representation, a pair of opposite charges lacked by the delocalized representation.

10. The method of claim 1, further comprising:
including, in the produced fixed bond representation, a pair of radicals lacked by the delocalized representation.

Sub 4 11. The method of claim 1, further comprising:-
queueing at least a subset of the candidates by priority.

Sub 5 12. The method of claim 1, further comprising:
using a precomputed table of atom valences as a function of element, charge, radical state, and number and distribution of bonds inside and outside of a delocalized region in the delocalized representation.

Sub 6 13. The method of claim 1, wherein the table includes an extensible component.
14. The method of claim 1, wherein the table is extensible to apply to any chemical element.

Sub 7 15. The method of claim 1, further comprising:
deriving electronic state and valence distributions information together with analyzing the delocalized representation.

16. The method of claim 1, further comprising:
determining whether it is practicable to produce a fixed bond representation of the chemical structure.

Sub 8 17. The method of claim 1, further comprising:
determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of radicals requirements.

18. The method of claim 1, further comprising:

Q2 determining whether it is possible to produce a fixed bond representation of the chemical structure that meets a set of charges requirements.